

Entanglement Dynamics in Harmonic Oscillator Chains

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We study the long-time evolution of the bipartite entanglement in translationally invariant 1D harmonic lattice systems. We show that for a wide class of Hamiltonians and generic initial states there exists a *lower* bound for the von Neumann entropy which increases linearly in time. This implies that the dynamics of harmonic lattice systems can in general not efficiently be simulated by algorithms based on matrix-product decompositions of the quantum state.

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Recently, so-called matrix product states (MPS) have received much interest for the numerical simulation of one-dimensional quantum many body systems [1],[2]. This is because the ground state of fermionic and bosonic lattice systems with finite-range interactions and an excitation gap usually implies an area law of entanglement [3], stating that the von Neumann entropy of a partition scales with the surface size. In 1D the surface area is independent on the size of the system resulting in a weakly entangled ground state, which can thus faithfully be represented by MPS. Even when the excitation gap vanishes, i.e. for critical systems, there is only a correction which is at most logarithmic in the system size. The situation is however quite different for non-equilibrium problems as here not only the scaling with size but also with time is relevant. With respect to the latter only an upper bound derived by Lieb and Robinson exists [4], which states that the von Neumann entropy increases at most linear in time. Being an upper bound, it does of course not allow to draw any conclusion about the approximability of the long-time dynamics of quantum many-body systems by MPS. However, it is very often found, that the bi-partite entropy does indeed scale linear in time, which implies that the required computational resources increase exponentially in time. For example it has been shown for the spin- $\frac{1}{2}$ XY model that the entropy grows linearly with time after a global quench [5]. On the other hand, it was found recently for the case of free fermions that the entropy can grow only logarithmically in time [6], showing that for certain initial states the long-time dynamics is accessible with MPS based methods. If for free fermions the scaling of the entanglement entropy in time is only moderate for certain initial conditions, what kind of scaling with time can we expect for the entanglement entropy of free bosons?

In the present paper we study the time evolution of the entropy in 1D bosonic systems that evolve under translationally invariant quadratic Hamiltonians with local or finite-range couplings. In order to separate the problem of size-scaling from the scaling with time, which is the subject of interest in this paper, we consider a specific class of 1D systems where the bi-partite entropy be-

comes independent on system size. To this end we choose as initial state of the time evolution the ground state Φ of some local, gapped Hamiltonian H_0 . As explained in the following, one can intuitively expect that under such initial conditions the bi-partite entanglement entropy of the time-evolved state will be independent on system size. Since for the ground state of local Hamiltonians the presence of an excitation gap is sufficient for an area law of entanglement [3], the entropy of the initial state is size independent. It is easy to see that the state time-evolved under a Hamiltonian H , $\Psi(t) = \exp\{-iHt\}\Phi$, is the ground state of a time-dependent Hamiltonian $H'[t] = \exp\{-iHt\}H_0\exp\{iHt\}$. The spectrum of $H'[t]$ is identical to that of H_0 , i.e. it too has an excitation gap. Furthermore the Lieb-Robinson bounds guarantee that for any fixed time t its coupling matrix elements between sites i and j are exponentially small beyond a certain distance l_c , i.e. for $|i-j| > l_c$. Thus $H'[t]$ is also of finite range [7]. As a consequence we can expect that the entanglement entropy of the time-evolved state will saturate with increasing system size. However it is not possible to draw any conclusion about the time-scaling of entanglement beyond the limits set by the Lieb-Robinson *upper* bounds.

In the present paper we show that in contrast to free fermions the entropy of the time evolved quantum state *always* grows linearly in time, making a long-time simulation of 1D bosonic systems with MPS based methods impossible.

Translationally invariant harmonic oscillators: To be specific we consider a one-dimensional system of N bosonic oscillators described by N pairs of canonical operators $\mathbf{x} = (x_1, x_2, \dots, x_N)$ and $\mathbf{p} = (p_1, p_2, \dots, p_N)$. The oscillators are coupled by a quadratic Hamiltonian of the form

$$H = \frac{1}{2}\mathbf{p}^2 + \frac{1}{2}\langle \mathbf{x} | V | \mathbf{x} \rangle, \quad (1)$$

where V is a real, symmetric, positive definite, time-independent matrix. We assume translational invariance, implying that V is a Toeplitz matrix. Furthermore we consider periodic boundary conditions, such that V is

circulant. Circulant matrices form a commutative algebra. Moreover the elements of a circulant matrix can be generated from the spectral function $\lambda(\theta)$, i.e.

$$V_{kl} = \frac{1}{2\pi} \int_0^{2\pi} d\theta \lambda(\theta) e^{-i(k-l)\theta}. \quad (2)$$

We now want to determine the scaling of the entanglement entropy with time. To this end we have to find the time evolution under the local Hamiltonian (1). The system is assumed to start its evolution at $t = 0$ from a Gaussian state, i.e.

$$\Phi(\mathbf{x}) = \alpha_0 \exp\left(-\frac{1}{2} \langle \mathbf{x} | B | \mathbf{x} \rangle\right), \quad \alpha_0 = \left(\frac{\det B}{\pi^N}\right)^{1/4} \quad (3)$$

where B is a real, symmetric, and positive definite Toeplitz matrix. Periodic boundary conditions imply that B is also a circulant matrix with spectral function $\beta(\theta)$. As the initial state is the ground state of a gapped, local Hamiltonian, $\beta(\theta)$ is non-zero and regular corresponding to a non-critical state. Since the Hamiltonian of the system is quadratic, the time-evolved state remains Gaussian and we have to search for a solution in the form

$$\Psi(\mathbf{x}, t) = \frac{1}{(\pi^N \det \tilde{A}^{-1})^{1/4}} \exp\left(-\frac{1}{2} \langle \mathbf{x} | A(t) | \mathbf{x} \rangle\right). \quad (4)$$

Here and in the following a tilde denotes the real part, i.e. $\tilde{X} = \frac{X+X^*}{2}$. By taking into account the symmetry of B and after simple calculations one can easily find that $A(t)$ obeys the Riccati equation

$$i \frac{\partial A}{\partial t} = A^2 - V, \quad A(0) = B. \quad (5)$$

Its solution can be written as

$$A(t) = V^{1/2} \frac{\cos(tV^{1/2}) B + iV^{1/2} \sin(tV^{1/2})}{\cos(tV^{1/2}) V^{1/2} + i \sin(tV^{1/2}) B} \quad (6)$$

which is again a circulant matrix. The spectral function $\Lambda(\theta, t)$ of its real part \tilde{A} can easily be obtained from $\lambda(\theta)$ and $\beta(\theta)$:

$$\Lambda(\theta, t) = \frac{\beta(\theta) \lambda(\theta)}{\lambda(\theta) \cos^2(t\lambda^{1/2}(\theta)) + \beta^2(\theta) \sin^2(t\lambda^{1/2}(\theta))}, \quad (7)$$

Note that if $B = V^{1/2}$, the spectral function and thus the matrix $A(t)$ becomes time-independent, as in this case the initial state is the ground state of the full Hamiltonian.

Reduced density matrix: Having the solution of the Schrödinger equation we can now calculate the reduced density matrix of a block of $N - n$ oscillators. The calculations can be done by partitioning the symmetric matrices $A(t)$ and $A^{-1}(t)$ into blocks

$$A(t) = \begin{bmatrix} T & C \\ C^T & R \end{bmatrix}, \quad A^{-1}(t) = \begin{bmatrix} Q & D \\ D^T & P \end{bmatrix} \quad (8)$$

where T is an $n \times n$ and R an $(N - n) \times (N - n)$ matrix. Similar calculations have been done in [8] and [9] for the ground state of a chain of oscillators. After a lengthy but straightforward calculation we find for the matrix elements of the reduced density operator

$$\rho_R(\mathbf{x}, \mathbf{x}') = \mathcal{N} \exp \left[\begin{pmatrix} \mathbf{x} \\ \mathbf{x}' \end{pmatrix}^T \begin{bmatrix} -\Gamma & \Delta \\ \Delta^* & -\Gamma^* \end{bmatrix} \begin{pmatrix} \mathbf{x} \\ \mathbf{x}' \end{pmatrix} \right], \quad (9)$$

where $\mathbf{x} = (x_{n+1}, \dots, x_N)$, $\mathbf{x}' = (x'_{n+1}, \dots, x'_N)$ are the coordinates of the remaining $N - n$ oscillators,

$$\Gamma = \frac{R}{2} - \frac{C^T \tilde{T}^{-1} C}{4}, \quad \Delta = \frac{C^T \tilde{T}^{-1} C^*}{4},$$

and $\mathcal{N} = (\det \tilde{P}^{-1})^{1/2} / (\pi)^{\frac{N-n}{2}}$ is a normalization with

$$\tilde{P}^{-1} = \tilde{R} - \tilde{C}^T \tilde{T}^{-1} \tilde{C}, \quad (10)$$

Here and in the following \tilde{Y}^{-1} denotes $(\tilde{Y})^{-1}$.

Purity and lower bound for the Entropy: We proceed by analyzing the dynamical behavior of the bi-partite entanglement. There are several measures of entanglement between parties of a closed system, examples being the von Neumann entropy $S = -\text{tr}(\rho_R \ln \rho_R)$ and the purity $\text{tr} \rho_R^2$, where the following inequality holds $S \geq -\ln \text{tr}[\rho_R^2]$. It should be noted that $-\ln \text{tr} \rho_R^2$ represents also a lower bound to all Renyi entropies $S_\alpha = \frac{1}{1-\alpha} \ln \text{tr}[\rho_R^\alpha]$ with $\alpha < 1$ as $S_\alpha > S_1 = S$.

In order to derive a lower bound for the entropy we calculate the purity of (9).

$$\text{tr}[\rho_R^2] = \int d\mathbf{x} d\mathbf{x}' \rho_R(\mathbf{x}, \mathbf{x}') \rho_R(\mathbf{x}', \mathbf{x}). \quad (11)$$

The Gaussian nature of (9) allows to calculate this integral in a straight-forward way:

$$\text{tr}[\rho_R^2] = \frac{(\det \tilde{P}^{-1})}{(\det [\tilde{\Gamma} - \tilde{\Delta}] \det [\tilde{\Gamma} + \tilde{\Delta}])^{1/2}}. \quad (12)$$

After simple algebra one obtains

$$\text{tr}[\rho_R^2] = \left[\det \left(\tilde{P} \left(\tilde{R} + Z^T \tilde{T}^{-1} Z \right) \right) \right]^{-1/2} \leq \left[\det \left(\tilde{P} \tilde{R} \right) \right]^{-1/2},$$

where $Z = (C - C^*)/2i$. The last inequality follows from the fact that $Z^T \tilde{T}^{-1} Z$ is a positive definite matrix. With this we find the following lower bound to the von-Neumann entropy

$$S \geq \frac{1}{2} \ln \det \left(\tilde{P} \cdot \tilde{R} \right). \quad (13)$$

In order to facilitate analytical calculations of determinants, we consider the limits $N \gg 1$ and $N > n \gg 1$. It

can then be shown [10] that in this limit the elements of matrices \tilde{R} and \tilde{P} can be generated from the spectral functions $\Lambda(\theta, t)$ and $\Lambda^{-1}(\theta, t)$ respectively. As $\Lambda(\theta, t)$ is a regular function i.e. $\Lambda(\theta, t) > 0$ for any t , we may apply the strong Szegő theorem [11] to calculate the determinants. According to this theorem

$$S \geq \sum_{k=1}^{\infty} k |c_k|^2, \quad (14)$$

where the c_k are Fourier coefficients of $\ln \Lambda^{-1}(\theta, t)$, i.e.,

$$c_k = \frac{1}{2\pi} \int_0^{2\pi} d\theta \ln \Lambda^{-1}(\theta, t) \exp(-i\theta k). \quad (15)$$

If $\beta(\theta)$ and $\lambda(\theta)$ are constant function i.e. the oscillators are uncoupled, all Fourier coefficients (15) vanish except for c_0 . In this case (14) reduces to the trivial bound $S \geq 0$ (entanglement is never generated). In what follows we will consider only the non trivial case when $\lambda(\theta)$ is a not constant.

In Fig. 1 we have plotted the right hand side of eq.(14) numerically evaluated for an initial state with spectral function $\beta(\theta) = 1$ and a Hamiltonian H with spectral function $\lambda(\theta) = (c - \cos(\theta))^2$. If $c > 1$, H has a finite excitation gap as there are no real zeroth of $\lambda(\theta)$. If the gap vanishes, i.e. for $c \leq 1$ the ground state of H becomes critical. One clearly recognizes a linear increase with time in all cases. That the presence of an excitation gap is irrelevant here is not surprising, as the initial state has a finite overlap with excited states except in the trivial case where it coincides with the ground state.

For short times one should expect that the sum grows quadratically in time [12]. The spectral function $\Lambda(\theta, t)$ (7) for small t scales approximately quadratic in t

$$\Lambda(\theta, t) \approx \beta(\theta) [1 - (\beta^2(\theta) - \lambda(\theta)) t^2]. \quad (16)$$

The correction to the initial spectral function is proportional to difference $\beta^2(\theta) - \lambda(\theta)$, as was expected. The Fourier coefficients c_k (15) can then easily be calculated $c_k \approx \xi_k + t^2 \delta_k$, where ξ_k and δ_k are some constant numbers. From this one can calculate the sum (14) for short time which yields

$$S \geq \varkappa_1 + \varkappa_2 t^2 \quad (17)$$

In the following we will derive an analytic estimate for the lower bound to the entropy for large times. Note that $\beta^2(\theta) = \lambda(\theta)$ corresponds to an initial state that is an eigenstate of H and thus has no time evolution at all. In any real system, the number of oscillators in the chain is finite and therefore to neglect boundary effects in the thermodynamic limit it is necessary consider time intervals $t \leq L/v$, where v is the speed for excitations after a quench, the so-called Lieb-Robinson speed [4] (see also:

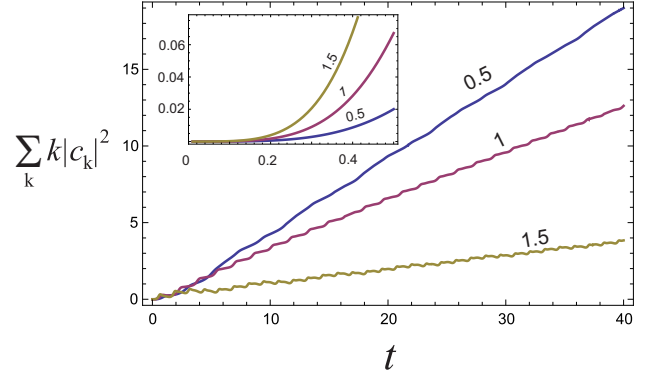


FIG. 1: (Color online) Numerical plot for the sum $\sum_{k=1}^{\infty} k |c_k|^2$ as function of time for a Hamiltonian H with spectral function $\lambda(\theta) = (c - \cos \theta)^2$ and for initial Gaussian state $\beta(\theta) = 1$. The top-most curve (blue) corresponds to the critical Hamiltonian with $c = 0.5$, the middle curve (magenta) to the critical Hamiltonian with $c = 1$, and the lowest curve (yellow) to a gapped Hamiltonian with $c = 1.5$. One clearly recognizes a linear increase with time. The insert shows the quadratic short-time evolution.

[7]), and L is the system size. For the sake of simplicity of the derivations we consider a Hamiltonian H with a finite excitation gap. The derivation for a non-gapped Hamiltonian is more involved and will not be presented here. As noted above the presence of a gap is however irrelevant. In the following we use an alternative expression for $\sum_{k=1}^{\infty} k |c_k|^2$ which is very useful for numerical and analytical calculations. By Parseval's theorem this sum can

$$\text{be rewritten as } \sum_{k=1}^{\infty} k |c_k|^2 = \frac{1}{8\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} d\eta_1 d\eta_2 \frac{\ln^2 \frac{\Lambda(\eta_1 - \eta_2, t)}{\Lambda(\eta_1 + \eta_2, t)}}{\sin^2 \eta_2}.$$

Making use of the inequality $\left| \ln \left| \frac{x}{y} \right| \right| > \frac{1}{M} ||x| - |y||$, $0 < |x|, |y| \leq M$ one finds

$$S > \frac{1}{M^2} \sum_{k=1}^{\infty} k |b_k|^2, \quad (18)$$

where $M = \max \Lambda(\theta, t)$, and

$$b_k = \frac{1}{2\pi} \int_0^{2\pi} d\theta \Lambda^{-1}(\theta, t) \exp(-i\theta k). \quad (19)$$

The coefficients b_k have a simple physical meaning: They determine the correlations in momentum space over a distance k , i.e. $\langle \Psi(t) | p_i p_{i+k} | \Psi(t) \rangle \sim b_k$. With this we have

$$S > \frac{1}{M^2} \sum_{k=1}^{\infty} k (\varsigma_k + \mu_k(t))^2 \quad (20)$$

where we have decomposed $\Lambda^{-1}(\theta, t)$ in a time indepen-

dent and a time dependent term

$$s_k = \frac{1}{4\pi} \int_0^{2\pi} d\theta \frac{\lambda(\theta) + \beta^2(\theta)}{\beta(\theta)\lambda(\theta)} \cos(k\theta), \quad (21)$$

$$\mu_k(t) = \frac{1}{4\pi} \int_0^\pi d\theta \frac{\lambda(\theta) - \beta^2(\theta)}{\lambda(\theta)\beta(\theta)} \cos\left(2t\lambda^{1/2}(\theta)\right) \cos(k\theta). \quad (22)$$

The term proportional to ζ_k^2 in eq.(20) does not depend on time and can be disregarded. The second term can be rewritten using the triangular inequality and Parseval theorem to give $\left| \sum_{k=1}^\infty k \zeta_k \mu_k(t) \right| \leq \left[\sum_{k=1}^\infty k \zeta_k^2 \sum_{k=1}^\infty k \mu_k^2(t) \right]^{1/2} = \left[C_1 \sum_{k=1}^\infty k \mu_k^2(t) \right]^{1/2}$. The time dependence of this term is thus given by the square root of the term containing $\mu_k(t)^2$.

We now show that the term $\sim \mu_k(t)^2$ in eq.(20) is bounded from below by a function linear in t . To this end we evaluate the integral in eq.(22) for $\mu_k(t)$ by the method of stationary phase (the role of the large parameter is played by t). The stationary points of the phase $2\lambda^{1/2}(\theta) \pm \frac{k}{t}\theta$ are the solution of

$$\frac{1}{\lambda^{1/2}(\theta, t)} \frac{d\lambda(\theta, t)}{d\theta} \pm \frac{k}{t} = 0. \quad (23)$$

As the interaction matrix V is of finite range, the spectral function $\lambda(\theta)$ is a trigonometric polynomial of finite degree K . By the theorem of Bernstein [11] one has $\max \left| \frac{d\lambda(\theta)}{d\theta} \right| \leq K \max \lambda(\theta)$, and therefore if $k \geq k_{\max} = \frac{K \max \lambda(\theta)}{\sqrt{\min \lambda(\theta)}} t = v_g t$ eq. (23) has no real solutions. For these values of k all $\mu_k(t)$ are exponentially small in agreement with the finite Lieb-Robinson speed. On the other hand, when t and k are large but $k \leq v_g t$ one finds

$$\mu_k(t) \approx \frac{1}{\sqrt{t}} \sum_{m=1}^W F_m\left(\frac{k}{t}\right) \cos\left(t G_m\left(\frac{k}{t}\right) + \varphi_m\right), \quad (24)$$

where $F_m\left(\frac{k}{t}\right)$ and $G_m\left(\frac{k}{t}\right)$ are some "nice" functions. $F_m\left(\frac{k}{t}\right)$ is proportional to $\int d\theta [\lambda(\theta) - \beta^2(\theta)]$ which quantifies the difference between initial state and ground state of H . If both agree, i.e. if $\beta(\theta)^2 = \lambda(\theta)$, the coefficient vanishes. The integer W is the number of stationary points, which must be finite because $\lambda(\theta)$ is a trigonometric polynomial of finite degree. $\varphi_m = \pm \frac{\pi}{4}$ depending of the sign of the second derivative of $\lambda^{1/2}(\theta)$ at the stationary points. Thus $\sum_{k=1}^\infty k \mu_k^2(t) > \sum_{k=1}^{v_g t} k \mu_k^2(t) \approx \sum_{k=1}^{v_g t} \frac{k}{t} \left| \sum_{m=1}^W F_m\left(\frac{k}{t}\right) \cos\left(t G_m\left(\frac{k}{t}\right) + \varphi_m\right) \right|^2$ By replacing summation by integration and neglecting all

highly oscillating terms we arrive at

$$\sum_{k=1}^\infty k \mu_k^2(t) > \frac{t}{2} \int_0^{v_g} dx x \sum_{m=1}^W F_m(x)^2 = \alpha_2 t + \mathcal{O}(t^{1/2}).$$

Thus

$$S > C t, \quad (25)$$

with

$$C = \frac{1}{2M^2} \int_0^{v_g} dx x \sum_{m=1}^W \left(F_m(x)\right)^2 \quad (26)$$

being a finite time-independent constant. Eq.(25) is the main result of our paper. It constitutes a lower bound to the scaling of the entanglement entropy $S_\alpha, \alpha \leq 1$ with time in a one-dimensional system of coupled harmonic oscillators. Eq.(25) implies that the bond dimension of the matrices used in an MPS representation needs to increase exponentially in time to allow for a faithful representation of the dynamical many body wavefunction. This means that in contrast to fermionic systems, where at least for certain initial conditions a simulation of the long-time dynamics is possible, for harmonic oscillator systems this is in general impossible. The discussion can be extended to d dimensions. In higher dimensions the form of the reduced density matrix is the same as Eq.(9). To calculate determinants of Toeplitz matrices one can apply the d -dimensional Szegő theorem [13].

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